REMARKS/ARGUMENTS

The office action issued May 20, 2005 continues the rejection of claim 1 under 35 U.S.C. § 102(b). Claims 2-7 were allowed.

The Examiner has rejected claim 1 under 35 U.S.C. 102(b): "... as being anticipated by International Application Publication Number WO 99/44055 to Nicholls." Specifically, the Examiner states:

> With regard to claim 1 Nicholls discloses a computer implemented method to search a heterogeneous compound database composed of molecules from different sources and syntheses, some known and some unknown, for molecules which have the same biological activity as a known query molecule (see abstract) comprising the steps of fragmenting a query molecule and a database molecule according to a defined set of rules (see page 10 line 25), generating shape descriptors for the query molecule and database molecule fragments (see page 22 line 10-19), and using the shape descriptors identifying the database molecule which has a shape similar to the query molecule (see page 25 line 5-26).

In response to the arguments previously presented by Applicants with respect to claim 1, the Examiner states:

> Applicant's arguments filed 4-6-2005 have been fully considered but they are not persuasive.
>
> In response to applicant's argument regarding claim 1 that the references fail to show certain features of applicant's invention, it is noted that the features upon which

applicant relies (i.e., matching a "whole" query molecule) are not recited in the rejected claim(s). Although the claims are interpreted in light of the specification, limitations from the specification are not read into the claims. See *In re Van Geuns*, 988 F.2d 1181,26 USPQ2d 1057 (Fed. Cir. 1993).

Applicants' Response:

Applicants respectfully continue to believe that the Examiner's analysis is incorrect and present the following further arguments. Initially, Applicants note that the Examiner is correct in having considered Nicholls since Nicholl's goal is in some respects similar to Applicants' goal. However, Nicholl's approach differs substantially from that of Applicants'. In their prior response, Applicants focused on only one aspect of the difference between Nicholls and Applicants since that aspect alone is sufficient to rule out Nicholls as anticipating Applicants' invention. In fact, Nicholls substantially differs from Applicants' invention in other significant ways. As an example, Nicholls approximates the shape of a molecule or molecular fragment using ellipsoidal Gaussian functions:

> My approach is simple and yet quite powerful. I seek to represent the molecular field by certain simpler shapes, namely ellipsoidal Gaussian functions (EGF). An EGF is a mathematical form that specifies a value at each point in space that is equal to: p*exponential of (-a*x*x-b*y*y-c*z*z) where x, y and z are distances in mutually orthogonal directions from a particular point in space, a, b and c are positive constants, and p may be positive or negative but is usually positive. This function falls off rapidly far from its center and has the symmetry of an ellipsoid. (starting at line 23, page 28)

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Applicants do not use this approach. Instead, Applicants teach the use of the topomeric

alignment of molecular fragments. The topomeric alignment aligns molecular fragments in a

uniform manner so that their shapes can be usefully compared. Applicants utilize the fields

around the topomericallly aligned fragments as their shape comparison metric. They do not use

ellipsoidal Gaussian functions. Applicants submit that these differences alone preclude Nicholls

from anticipating Applicants' invention.

In view of Applicants' arguments distinguishing Applicants' invention from Nicholl's

presented in the prior response, the Examiner suggests that the feature (matching a "whole"

query molecule) upon which applicants rely to distinguish Nicholls is not recited in the rejected

claim. Applicants respectfully disagree. As noted in a different section of Applicants' prior

Response, in the normal course of usage as understood in the art, reference to a molecule is a

reference to the molecule as a whole molecule. Unless one specifically talks about parts or

fragments of a molecule as is done both in the present application and in the cited reference

(where Nicholls talks about "fragments, submolecules, and subfragments"), it is submitted that

the normal understanding of the word "molecule" is understood to mean the entire or whole

molecule.

This meaning of the word molecule to mean a whole molecule is used in a consistent

manner throughout claim 1. For instance, in the preamble:

A computer implemented method to search a heterogenous compound database composed

of molecules from different sources and syntheses, some known and some unknown, for

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molecules which are likely to have the same biological activity as a known query

molecule comprising the following steps:

Clearly, the meaning of molecule in the preamble refers to a whole molecule whether it be a

database molecule or a query molecule. Further in step a), fragmenting is used to mean the

breakup of whole molecules either database molecules or query molecule;

  fragmenting a query molecule and a database molecules according to a defined set of

  rules;

Finally, in step c), it is within the normal accepted usage of the word molecule to essentially read

the step as meaning:

  c) using the shape descriptors, identifying the *whole* database molecule which has a

  shape similar to the *whole* query molecule. (bold text for emphasis only)
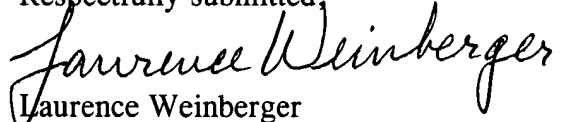
Applicants respectfully submit that the feature upon which they relied when making their

argument in the prior response, namely that Applicants' method matched a "whole"query

molecule is properly recited given the standard term of art meaning of the word molecule.

Applicants submit that Applicants have properly claimed their invention and, for the reasons

fully set out in Applicants' prior response, which is fully incorporated herein, that Nicholls

does not anticipate Applicants' invention.

  For all the reasons stated above, Applicants submit that Nicholls does not anticipate

Applicants' invention. Applicants respectfully request that the Examiner withdraw the rejection

of record to claim 1 and permit the application to issue.

Respectfully submitted,

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